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14. ABSTRACT The goal of this project is to develop a fundamental understanding of how fluid flows, electric fields, and surface patterning affect polyelectrolyte adsorption, self-assembly, and transport near solid surfaces. Polyelectrolytes are charged polymers whose behavior is central to Army-relevant technologies (e.g., biochemical sensors, surface functionalization) but poorly understood. Brownian dynamics simulations---a coarse-grained simulation method suitable for describing non-equilibrium polymer behavior---have been applied to study polyelectrolyte adsorption in shear flow, polyelectrolyte adsorption onto patterned surfaces, dendrimer and hyperbranched polymer adsorption, and polyelectrolyte electrophoresis. Along with					
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Report Title

Dynamic Multiscale Simulation of Polyelectrolyte Nanoassemblies

ABSTRACT

The goal of this project is to develop a fundamental understanding of how fluid flows, electric fields, and surface patterning affect polyelectrolyte adsorption, self-assembly, and transport near solid surfaces. Polyelectrolytes are charged polymers whose behavior is central to Army-relevant technologies (e.g., biochemical sensors, surface functionalization) but poorly understood. Brownian dynamics simulations---a coarse-grained simulation method suitable for describing non-equilibrium polymer behavior---have been applied to study polyelectrolyte adsorption in shear flow, polyelectrolyte adsorption onto patterned surfaces, dendrimer and hyperbranched polymer adsorption, and polyelectrolyte electrophoresis. Along with complementary continuum-level models, the simulations yield insight into how to design fluid flows, electric fields, and surface patterning to control the behavior of single polyelectrolyte molecules. The knowledge gained lays the foundation for future studies involving multiple molecules and more complex physical phenomena.

List of papers submitted or published that acknowledge ARO support during this reporting period. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

1. S. H. Kim, A. S. Panwar, S. Kumar, K. H. Ahn, and S. J. Lee, "Electrophoresis of a Bead-rod Chain through a Narrow Slit: A Brownian Dynamics Study," J. Chem. Phys. 121, 9116-9122 (2004).
2. A. S. Panwar and S. Kumar, "Brownian Dynamics Simulations of Polyelectrolyte Adsorption in Shear Flow," J. Chem. Phys. 122, 154902 (12 pages) (2005).
3. A. S. Panwar and S. Kumar, "Time Scales in Polymer Electrophoresis through Narrow Constrictions: A Brownian Dynamics Study," Macromolecules 39, 1279-1289 (2006).
4. S. A. Roberts and S. Kumar, "Stability of Creeping Couette Flow of a Power-law Fluid past a Deformable Solid," J. Non-Newtonian Fluid Mech. 139, 93-102 (2006).
5. N. Hoda and S. Kumar, "Brownian Dynamics Simulations of Polyelectrolyte Adsorption onto Charged Patterned Surfaces," Langmuir 23, 1741-1751 (2007).
6. B. Suman and S. Kumar, "Adsorption of Charged Dendrimers: A Brownian Dynamics Study," J. Phys. Chem. B 111, 8728-8739 (2007).
7. N. Hoda and S. Kumar, "Kinetic Theory of Polyelectrolyte Adsorption in Shear Flow," J. Rheol. 51, 799-820 (2007).
8. N. Hoda and S. Kumar, "Brownian Dynamics Simulations of Polyelectrolyte Adsorption onto Topographically Patterned Surfaces," Langmuir 23, 11747-11760 (2007).
9. N. Hoda and S. Kumar, "Brownian Dynamics Simulations of Polyelectrolyte Adsorption in Shear Flow with Hydrodynamic Interaction," J. Chem. Phys. 127, 234902 (15 pages) (2007).
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(b) Papers published in non-peer-reviewed journals or in conference proceedings (N/A for none)

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(c) Presentations

1. A. S. Panwar (speaker) and S. Kumar, "Brownian Dynamics Simulations of Polyelectrolyte Adsorption in Shear Flow," 2004 Annual Meeting of the American Institute of Chemical Engineers, Austin, TX.
2. A. S. Panwar (speaker) and S. Kumar, "Brownian Dynamics Simulations of Polyelectrolyte Adsorption in Shear Flow," 2005 Annual March Meeting of the American Physical Society, Los Angeles, CA.
3. S. H. Kim, A. S. Panwar, S. Kumar, K. H. Ahn, and S. J. Lee, "Electrophoresis of a Bead-rod Chain through a Narrow Slit: A Brownian Dynamics Study," 2005 Annual March Meeting of the American Physical Society, Los Angeles, CA.
4. A. S. Panwar and S. Kumar, "Brownian Dynamics Simulations of Polymer Behavior in Microfluidic Systems," 2005 Gordon Research Conference on the Physics & Chemistry of Microfluidics, Oxford, United Kingdom (poster).
5. A. S. Panwar and S. Kumar, "Time Scales in Polymer Electrophoresis through Narrow Constrictions: A Brownian Dynamics Study," 2005 Annual Meeting of the American Institute of Chemical Engineers, Cincinnati, OH.
6. A. S. Panwar and S. Kumar (Invited), "Brownian Dynamics Simulations of Polyelectrolyte Adsorption in Shear Flow," 2006 Spring National Meeting of the American Chemical Society, Atlanta, GA.
7. S. Kumar (Invited), "Brownian Dynamics Simulations of Polymers: Modeling Long Molecules for Long Times," Army High Performance Computing Research Center/Army Research Laboratory Multidisciplinary Workshop on Verification and Validation (2006), Aberdeen, MD.
8. N. Hoda (speaker) and S. Kumar, "Brownian Dynamics Simulations of Polyelectrolyte Adsorption onto Charged Patterned Surfaces," 2006 Annual Meeting of the American Institute of Chemical Engineers, San Francisco, CA.
9. S. A. Roberts (speaker) and S. Kumar, "Stability of Creeping Couette Flow of a Power-law Fluid past a Deformable Solid," 2006 Annual Meeting of the American Physical Society Division of Fluid Dynamics, Tampa, FL.
10. N. Hoda (speaker) and S. Kumar, "Brownian Dynamics Simulations of Polyelectrolyte Adsorption onto Topographically Patterned Surfaces," 2007 Annual Meeting of the American Institute of Chemical Engineers, Salt Lake City, UT.
11. N. Hoda (speaker) and S. Kumar, "Polyelectrolyte Adsorption in Shear Flow with Hydrodynamic Interactions: Kinetic Theory and Brownian Dynamics Simulations," 2007 Annual Meeting of the American Institute of Chemical Engineers, Salt Lake City, UT.
12. B. Suman (speaker) and S. Kumar, "Adsorption of Charged Dendrimers: A Brownian Dynamics Study," 2007 Annual Meeting of the American Institute of Chemical Engineers, Salt Lake City, UT.

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Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

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Peer-Reviewed Conference Proceeding publications (other than abstracts):

1. S. Kumar (Keynote lecture), "Brownian Dynamics Simulation of Polymer Behavior in Nano- and Microfluidic Systems," in Proceedings of the 2004 International Conference on Computational & Experimental Engineering & Sciences, Madeira, Portugal, July 26-29, 2004, 1469-1472.
2. S. Kumar (Keynote lecture), "Brownian Dynamics Simulations of Polymer Behavior in Nanofluidic and Microfluidic Systems," in Proceedings of the Fifth International Conference on Nanochannels, Microchannels and Minichannels, Puebla, Mexico, June 18-20, 2007, ICNMM2007-30162 (3 pages).
3. N. Hoda and S. Kumar, "Polyelectrolyte Adsorption in Shear Flow with Hydrodynamic Interaction: Kinetic Theory and Brownian Dynamics Simulations," in AIP Conference Proceedings Volume 1027, The XVth International Congress on Rheology, Monterey, CA, August 3-8, 2008, 968-969.

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3

(d) Manuscripts

1. B. Suman and S. Kumar, "Brownian Dynamics Simulations of Hydrophobic Dendrimer Adsorption," accepted, Mol. Simul.

2. N. Hoda and S. Kumar, "Parameters Influencing Diffusion Dynamics of an Adsorbed Polymer Chain," submitted, Phys. Rev. Lett.

Number of Manuscripts: 2.00

Number of Inventions:

Graduate Students

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
Scott A. Roberts	0.20
Balram Suman	0.10
FTE Equivalent:	0.30
Total Number:	2

Names of Post Doctorates

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>	National Academy Member
Satish Kumar	0.10	No
FTE Equivalent:	0.10	
Total Number:	1	

Names of Under Graduate students supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period:	0.00
The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:.....	0.00
The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:.....	0.00
Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):.....	0.00
Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:	0.00
The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense	0.00
The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:	0.00

Names of Personnel receiving masters degrees

<u>NAME</u>
Total Number:

Names of personnel receiving PHDs

<u>NAME</u>
Ajay S. Panwar
Balram Suman
Nazish Hoda
Total Number:
3

Names of other research staff

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Sub Contractors (DD882)

Inventions (DD882)

Final Progress Report

Dynamic Multiscale Simulation of Polyelectrolyte Nanoassemblies

Satish Kumar, University of Minnesota

Statement of Problem Studied

Background

Polyelectrolytes are charged polymers (e.g., DNA and proteins) whose adsorption, self-assembly, and transport are poorly understood phenomena relevant to a number of important technologies such as biochemical sensors, nanofluidics and microfluidics, biocompatible coatings and materials, separation membranes, and microelectronic and photonic devices. The goal of this project is to develop a fundamental understanding of how fluid flows, electric fields, and surface patterning (chemical and/or topographical) affect polyelectrolyte adsorption, self-assembly, and transport near solid surfaces. Such fundamental understanding will enable the rational design of fluid flows, electric fields, and surface patterns for creation of polyelectrolyte nanoassemblies having tailored properties and for development of greatly improved polyelectrolyte separation processes. Beyond its intrinsic scientific importance, this project will significantly aid the Army in advancing its missions of developing new materials and materials processes, and establishing fundamental relationships between processing variables (here, fluid flows, electric fields, and surface patterning) and material behavior. This project also builds a solid theoretical underpinning for the technologies mentioned above (e.g., nanofluidics and microfluidics), which are of great interest to the Army and promise reduced costs, smaller weight and size, and higher reliability over existing technologies.

Brownian Dynamics Simulations

The principal tool used in this project is the Brownian dynamics simulation method. Brownian dynamics (BD) is a coarse-grained simulation method that is capable of describing polymer dynamics in non-equilibrium situations over relatively long time scales (~ 1 s). In BD, a polymer molecule is modeled as a series of beads connected by rigid rods (or flexible springs), while the solvent in which the polymer is immersed is taken to be a thermal bath that exerts random forces on the beads. The polymer dynamics are followed by integrating equations of motion for each bead, where the active forces are those due to viscous drag, the connectors between the beads, Brownian motion, externally applied flow and electric fields, and inter- and intra-molecular interactions. The expressions for each of these forces can be related to parameters that can be measured experimentally or calculated from finer-grained simulation methods such as molecular dynamics. BD simulations are carried out by performing a set of runs and then averaging over the ensemble to obtain properties of interest such as the conformations of molecules adsorbed to a surface and the velocity of a charged polymer in an electric field. Although BD uses a coarse-grained description of polymer molecules, it allows for simulations over time scales much longer than those that can be accessed by molecular dynamics simulations. Because many phenomena of interest in polyelectrolyte adsorption, self-assembly, and transport occur on such long time scales, BD is an ideal tool for studying them.

Below, we summarize our progress and accomplishments on several research problems related to the above project.

Summary of Most Important Results

Polyelectrolyte Adsorption in Shear Flow

In order to understand polyelectrolyte adsorption at a fundamental level, the logical place to start is the adsorption of single molecules. We performed the first molecular simulations of polyelectrolyte adsorption in shear flow [2], and were the first to incorporate hydrodynamic interaction (HI) into such simulations [9,11]. The key insight that comes out of these simulations is the discovery of a competition between polymer-surface attraction, which draws the polymer to the adsorbing surface, and polymer-surface HI, which drives the polymer away from the adsorbing surface. By combining the simulation results along with a kinetic theory [7], we were able to derive a scaling law relating the critical shear rate needed for desorption to various problem parameters.

Our results demonstrate how shear flow influences the adsorption of polyelectrolyte molecules, and show the critical role that HI plays. The simulation method and results of this work are expected to be useful for applications in which polyelectrolyte adsorption occurs in flowing fluids, such as biochemical sensors, nanofluidics and microfluidics, and biocompatible coatings and materials. Our efforts will lay the basis for future work in which we simulate the adsorption and self-assembly of multiple polyelectrolyte molecules onto a patterned surface in the presence of fluid flow. As most experiments involve multiple molecules, we expect that we will be able to compare predictions from our simulations with extensive experimental data already in the literature. The fundamental studies on single-molecule adsorption we have conducted will ultimately yield insight into how to design a flow field to achieve a polyelectrolyte nanoassembly with tailored properties.

Polyelectrolyte Adsorption onto Patterned Surfaces

Patterning of surface charge and topography is a powerful way to influence the conformations of adsorbed polymers. We performed the most comprehensive molecular simulations to date on polyelectrolyte adsorption onto surfaces decorated with periodic arrays of charged patches [5]. We also performed the first molecular simulations of polyelectrolyte adsorption onto topographically patterned surfaces [8]. The key insight that comes out of these studies is the discovery that the spatial structure of the electric field near the surface can have a significant impact on polymer conformations. This is in addition to any confinement effect due to the geometry of the charge or topographic patterns.

Our results demonstrate how polyelectrolyte conformations can be controlled by the design of surface charge and topography. Current work is focused on how dynamic properties, such as diffusion and rheology, are influenced by surface charge and topography [13]. We expect that our studies will be useful for applications where single chain adsorption is important such as sensors and biological processes, and also those where multiple chains may adsorb, such as polyelectrolyte multilayer formation. The

fundamental studies on single-molecule adsorption we have conducted will ultimately yield insight into how to design a surface to achieve a polyelectrolyte nanoassembly with tailored properties.

Dendrimer and Hyperbranched Polymer Adsorption

Whereas the simulations described above considered only linear polymers, polymers can have more complex architectures and these can be useful for applications such as surface functionalization, biochemical sensing, and drug delivery, all of which are of relevance to the Army. We performed the first BD simulations of dendrimer adsorption, considering both electrostatic [6] and non-electrostatic interactions [12]. Prior simulations of this phenomenon had been performed with either finer-grained simulation methods (molecular dynamics) or equilibrium methods (Monte Carlo). The coarse-grained nature of our simulations makes them much less computationally intensive than molecular dynamics simulations, and this enabled us to perform the first comprehensive investigation of how the distribution of charge and hydrophobicity within dendrimers influences adsorption behavior. The dynamic nature of our simulations allows us to probe non-equilibrium behavior in a rigorous way, overcoming a key limitation of Monte Carlo simulations.

Our results are expected to be helpful in providing qualitative guidance for dendrimer design in various applications, especially since it is extremely cumbersome to address the large parameter space involved through experiments alone. We are currently incorporating the effects of fluid flow, and then plan to consider more complex hyperbranched polymers (HBPs) and their self-assembly with nanoparticles for surface functionalization applications. These single-molecule studies will serve as a prelude to simulations in which we examine how multiple HBPs self-assemble with nanoparticles, and assembly behavior near surfaces and in fluid flows. Ultimately, we expect that the results of our work will help guide experimentalists to combinations of nanoparticles and HBPs which are promising for surface functionalization.

Polyelectrolyte Electrophoresis

Polyelectrolyte separations are a crucial component in biosensing, and are significantly influenced by the nature of the interactions between polyelectrolyte molecules and the surrounding surfaces, which may be patterned with charge and topography. We performed two BD studies of polyelectrolyte electrophoresis through narrow constrictions [1, 3]. Whereas previous studies examined transport in limiting cases where only one time scale is dominant, the major advance of our work is the elucidation of how multiple time scales can interact with each other. The results help explain existing experimental studies on DNA transport through entropic traps and nanopores. Future work will focus on incorporating HI into the simulations, examining how chemical patterning of the surfaces can be used to further control transport, and the effect of multiple polyelectrolyte molecules. It is important to emphasize that many of the tools and ideas developed in studying polyelectrolyte adsorption and self-assembly can be directly applied to study electrophoresis problems. We expect that the fundamental understanding gained from our studies will provide insight into how to design surfaces to

optimize polyelectrolyte separations, which in turn will advance the development of biosensors.

Continuum Modeling of Adsorption-related Phenomena

In addition to the molecular-level simulations described above, we also developed continuum-level models of various adsorption-related phenomena. Such models are valuable for several reasons. First, they can sometimes be formulated and solved quickly to obtain insight which can then be used to perform computationally intense molecular-level simulations more efficiently. Second, if the insights gained from molecular-level simulations can be distilled into a continuum-level model, then the model can serve as a convenient tool for prediction, design, and optimization in engineering applications. Third, by studying problems from both molecular- and continuum-level perspectives, knowledge can be gained about how to develop multiscale simulation tools that bridge the gap between small and large scales.

During this work, we developed several continuum-level models:

- The first kinetic theory of polyelectrolyte adsorption in shear flow [7]. The insight gained was instrumental in developing, validating, and interpreting the BD simulations discussed above, which can address situations too complex for the kinetic theory to handle.
- The first mean-field theory to study polyelectrolyte adsorption onto surfaces patterned with charge and topography [10]. The predictions of the theory provided considerable additional physical insight into the BD simulation results discussed above, which in turn can be used to reveal a number of phenomena beyond the scope of the theory.
- The first free-energy model of polyelectrolyte adsorption onto topographically patterned surfaces [8]. The model enabled us to rationalize the BD simulation results discussed above, and may be useful to other researchers in the field.
- The first linear stability analysis of a power-law fluid flowing past a soft polymer gel [4]. The analysis was motivated by the experimental observation that polyelectrolyte multilayers have rheological properties very similar to soft polymer gels. Since fluids flowing past soft polymer gels can become unstable and lead to degradation of the gel, multilayers may be susceptible to a similar degradation. Our analysis showed that instability is unlikely to occur for the range of problem parameters relevant to multilayer applications. Thus, if multilayer degradation in a fluid flow is observed experimentally, it will likely be because of a completely different physical mechanism.

Overall, these models complemented the knowledge obtained from our molecular simulations, deepened our physical understanding of the simulation results, and demonstrated how molecular- and continuum-level approaches can be combined in a synergistic way.

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1. S. H. Kim, A. S. Panwar, S. Kumar, K. H. Ahn, and S. J. Lee, "Electrophoresis of a Bead-rod Chain through a Narrow Slit: A Brownian Dynamics Study," J. Chem. Phys. 121, 9116-9122 (2004).
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8. N. Hoda and S. Kumar, "Brownian Dynamics Simulations of Polyelectrolyte Adsorption onto Topographically Patterned Surfaces," Langmuir 23, 11747-11760 (2007).
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12. B. Suman and S. Kumar, "Brownian Dynamics Simulations of Hydrophobic Dendrimer Adsorption," accepted, Mol. Simul.
13. N. Hoda and S. Kumar, "Parameters Influencing Diffusion Dynamics of an Adsorbed Polymer Chain," submitted, Phys. Rev. Lett.